Experimental measurement and Monte Carlo simulation of coherent interaction between high-energy particles and oriented crystals

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XXVI PhD course
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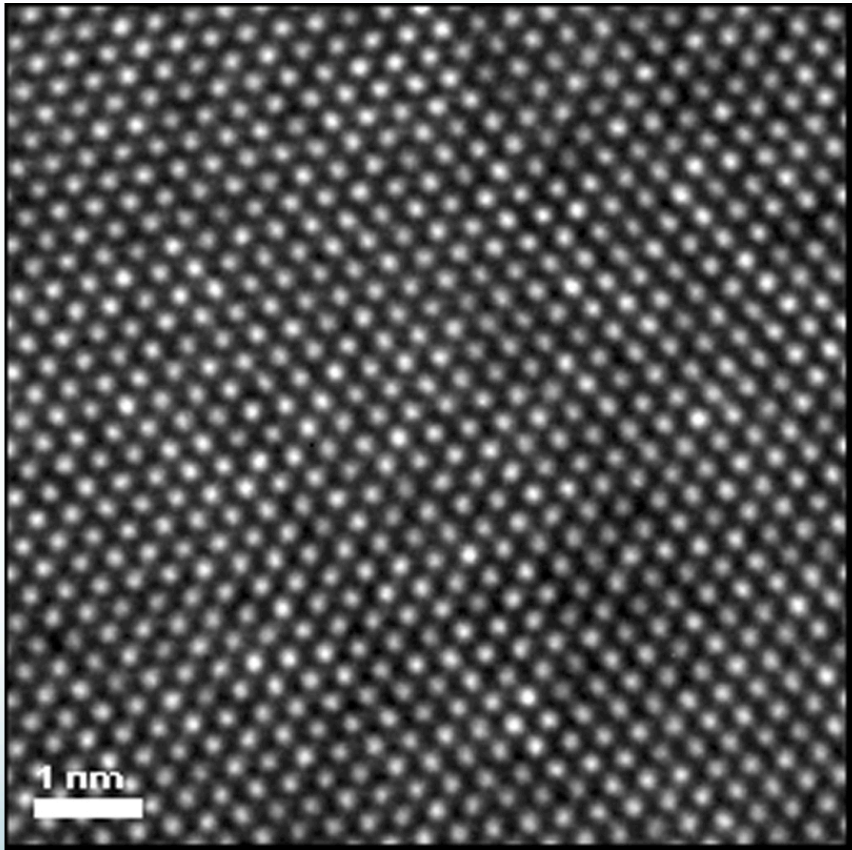
Outline

- High-energy coherent phenomena in crystals
- Experiments
  - 400 GeV/c protons:
    - Ge bent strip
    - Si crystalline undulator
    - Multi-crystals
    - SiGe self-bent crystal
  - 150 GeV/c π^-
    - Dechanneling length
- Monte Carlo
  - DYNECHARM++
  - DYNECHARM++_Phi
  - Geant4 Channeling

Channeling phenomenon

Crystal

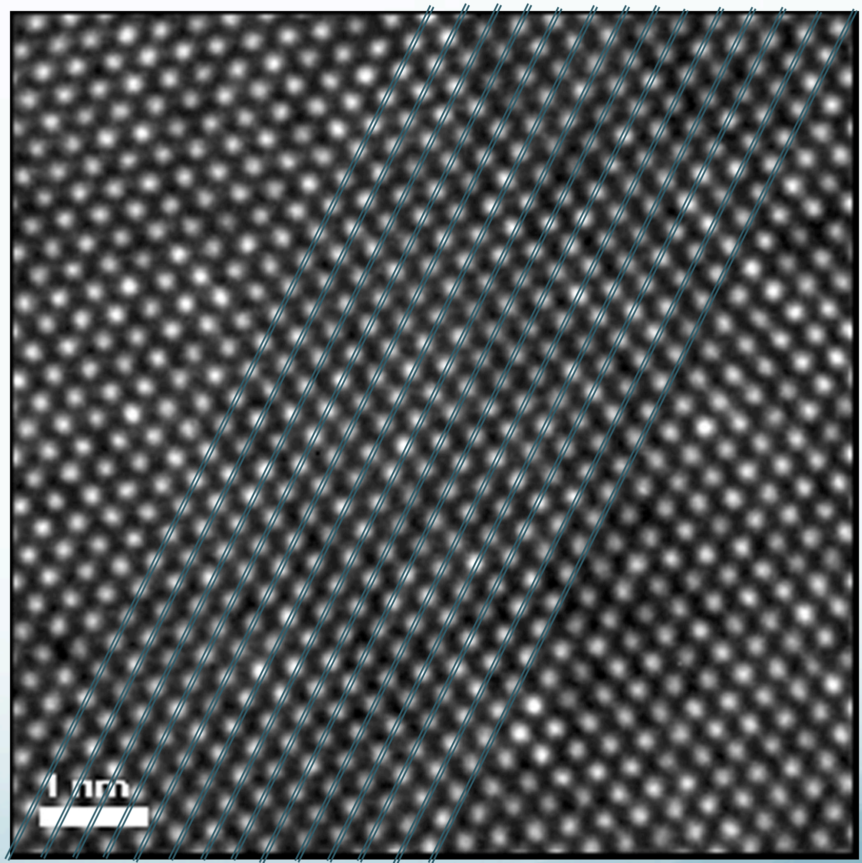
- Ordered pattern of atoms.



Ki-Bum Kim, SPIE Newsroom, DOI: 10.1117/2.1200812.1396

Crystal

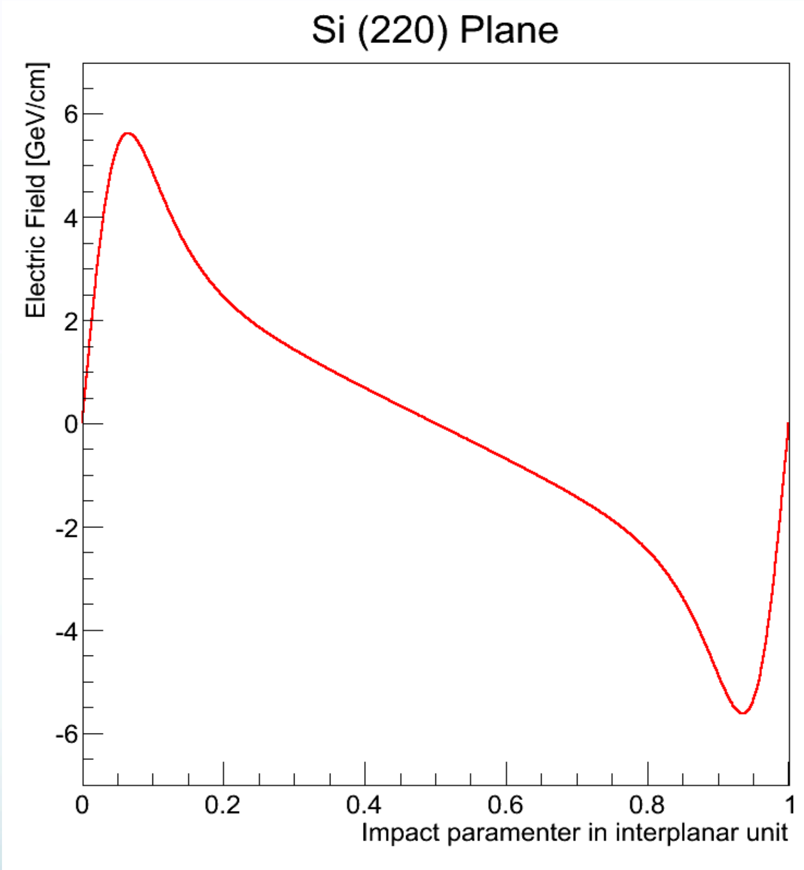
- Ordered pattern of atoms.
- Aligned atoms can be seen as planes or axes.



Ki-Bum Kim, SPIE Newsroom, DOI: 10.1117/2.1200812.1396

Crystal

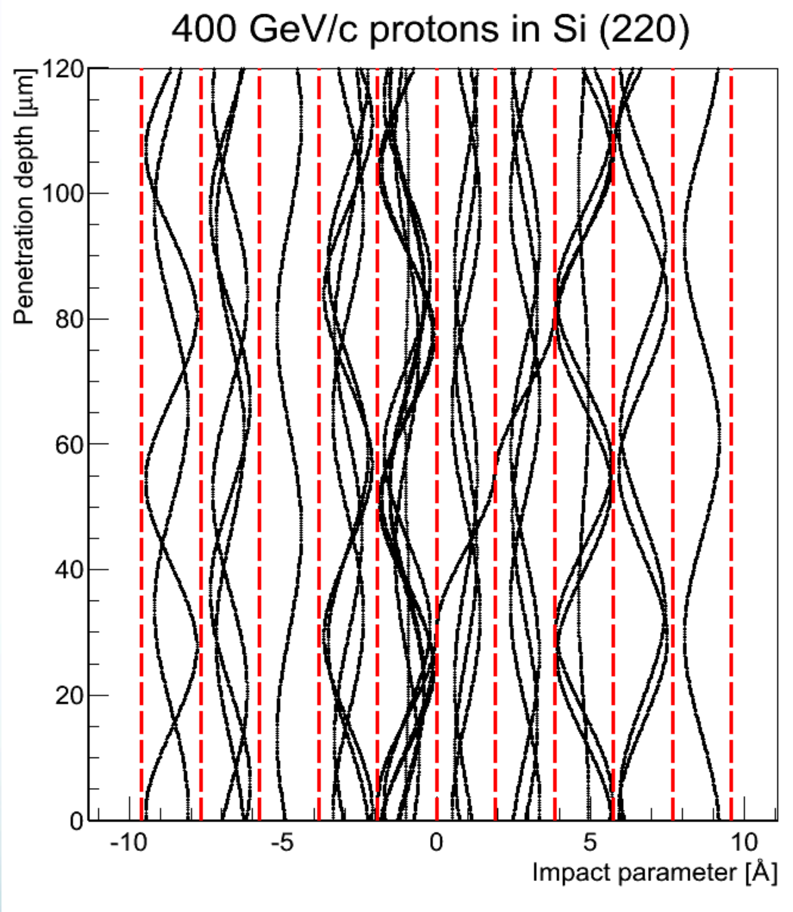
- Ordered pattern of atoms.
- Aligned atoms can be seen as planes or axes.
- Strong electromagnetic field between planes and between axes (GeV/cm).



ECHARM - E. Bagli, V. Guidi, V. A. Maisheev, PRE 81, 026708 (2010)

Crystal

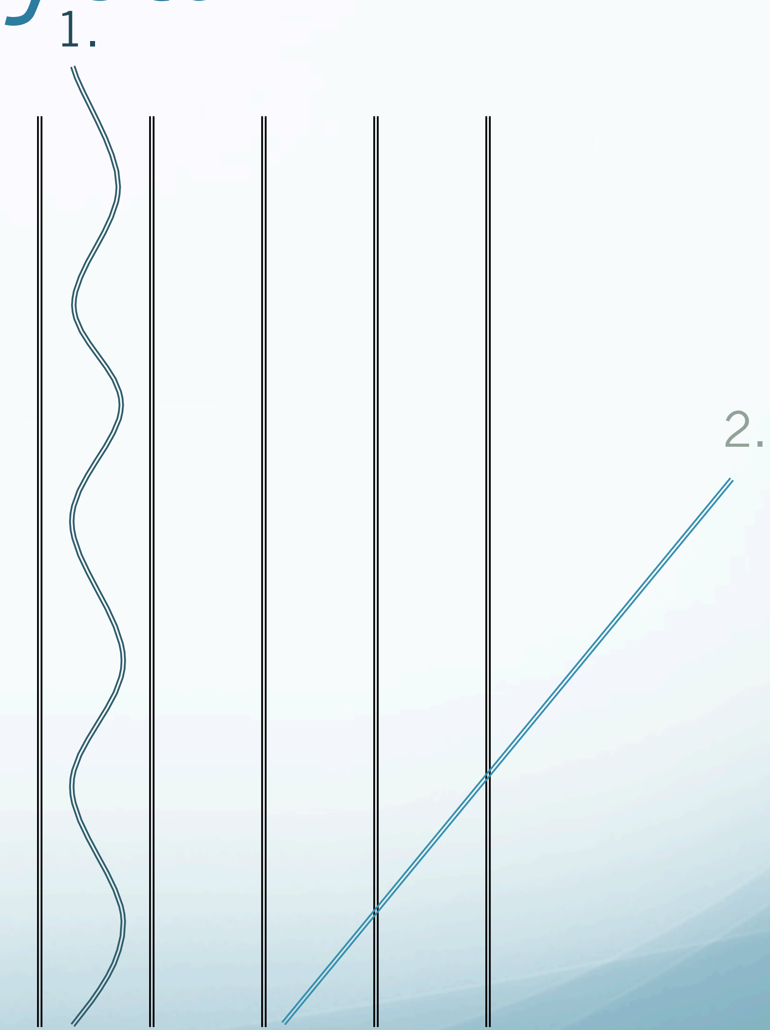
- Ordered pattern of atoms.
- Aligned atoms can be seen as planes or axes.
- Strong electromagnetic field between planes and between axes (GeV/cm).
- Channeling if particle direction



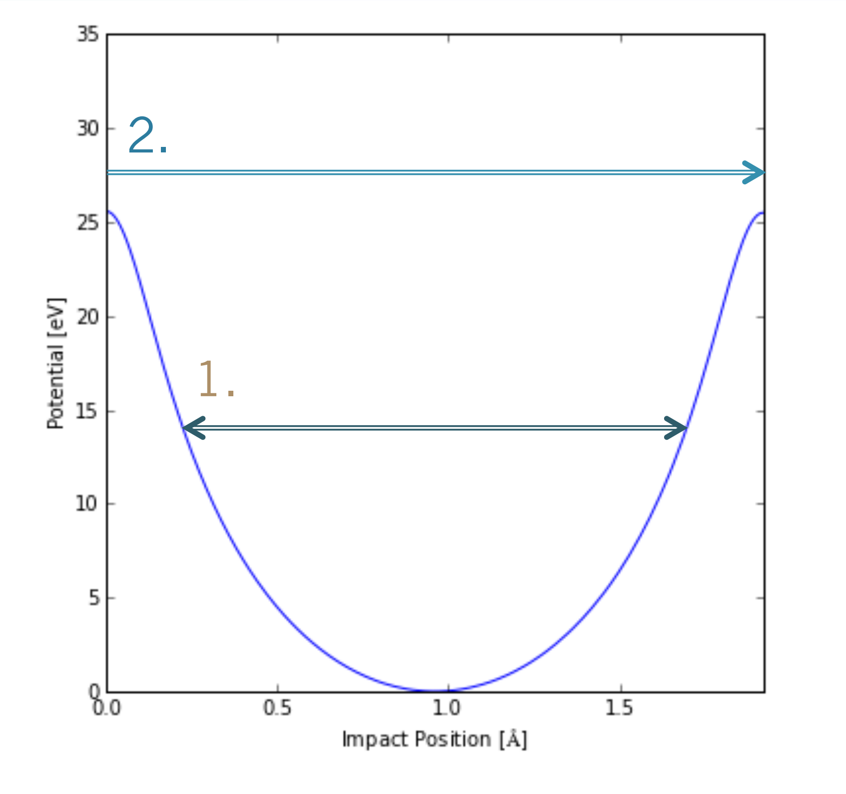
DYNECHARM++ - E. Bagli, V. Guidi, NIMB 309, 124 (2013)

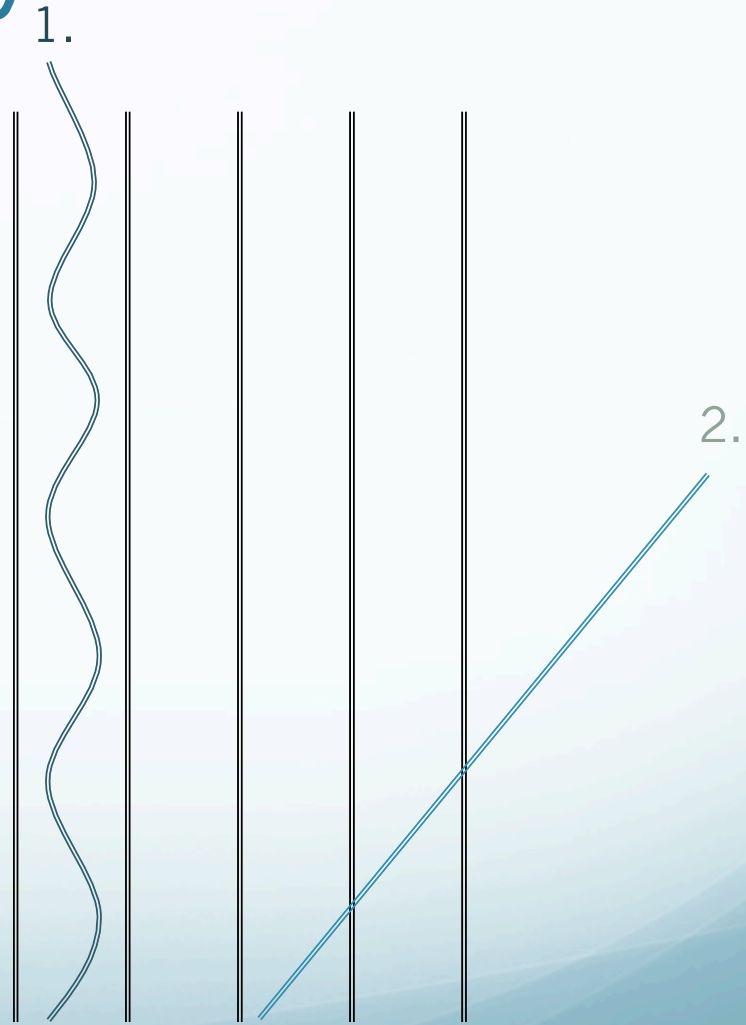
Straight crystal

- Particle whose direction of motion is aligned with crystal planes are captured in channeling.



Straight crystal

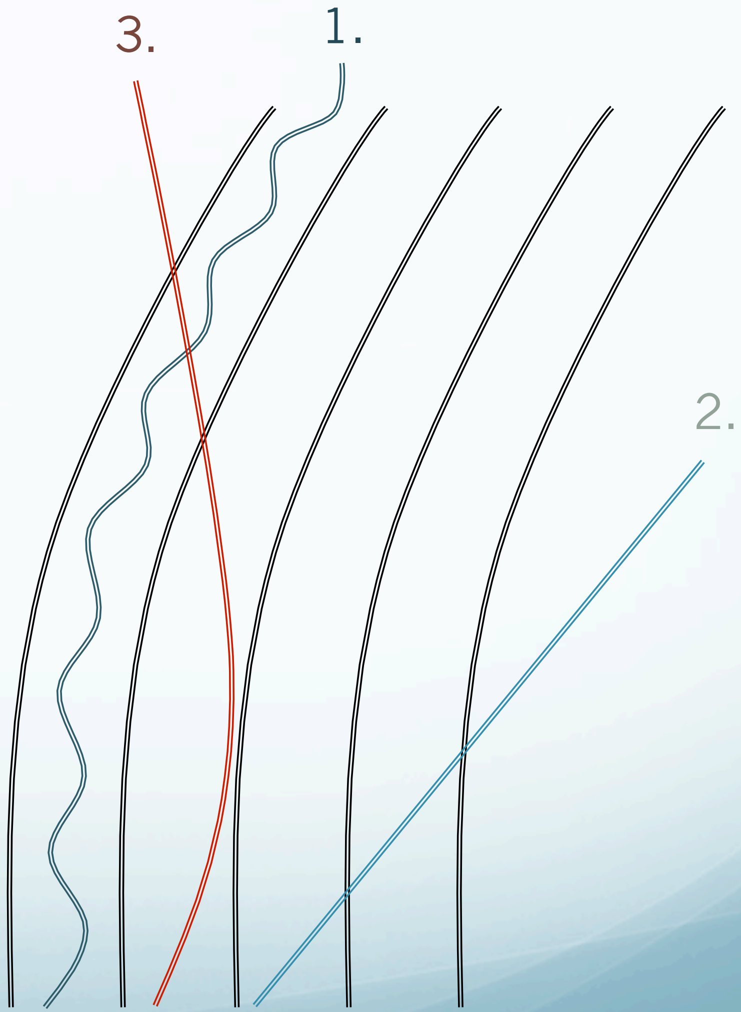




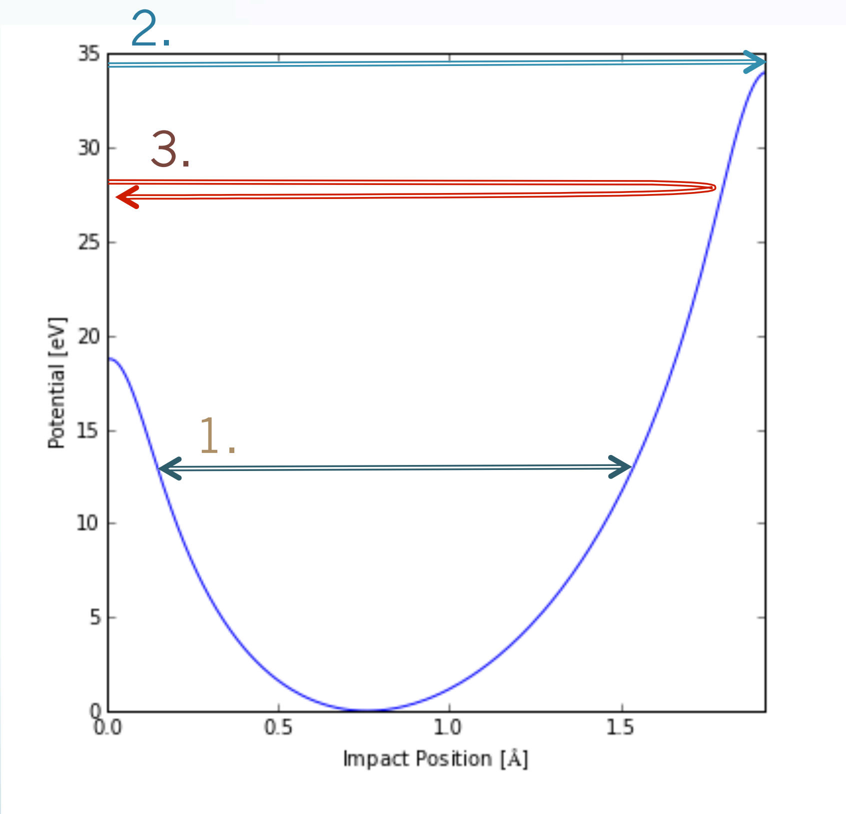
1. Channeled
2. Not channeled

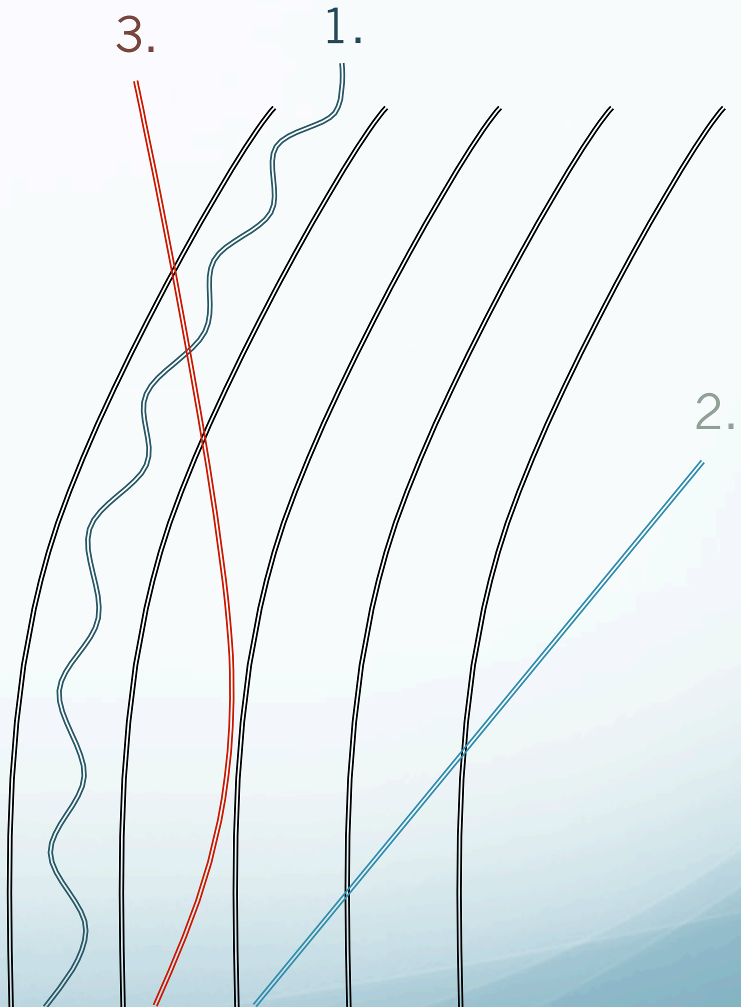
Bent crystal

- Channeled particles follows the crystal curvature and are deflected (1.).
- Particle whose trajectories is tangent to crystalline planes are "reflected" by the potential barrier (3.)



Bent crystal



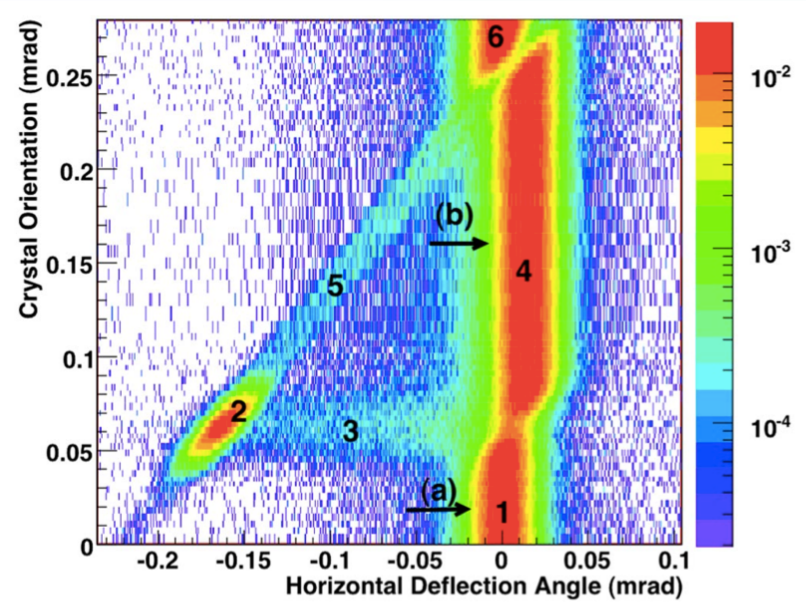


1. Channeled
2. Not channeled

Bent crystal

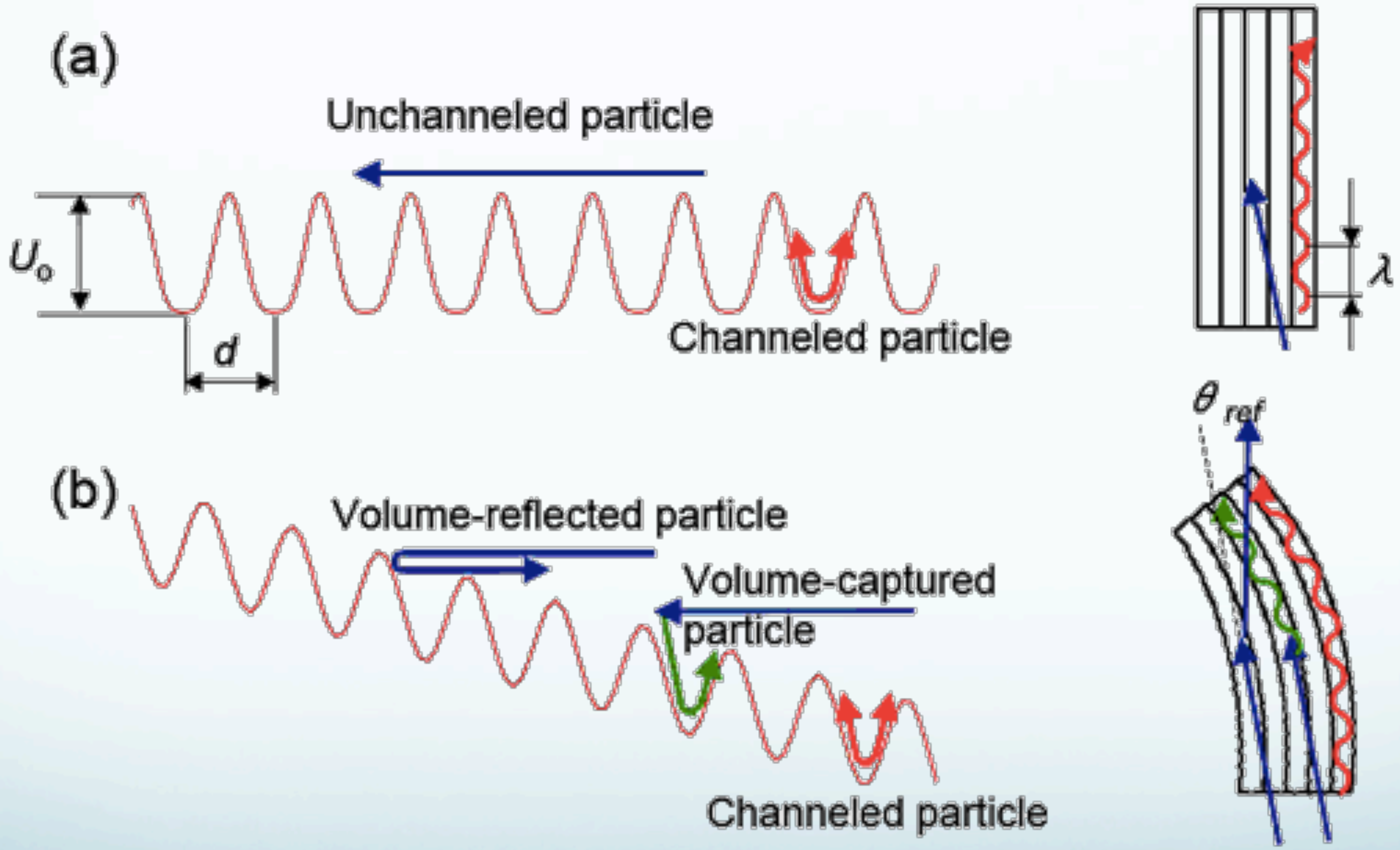
Varying the crystal orientation with respect to the beam direction orientational effects are observed:

1. No effect
2. Channeling
3. Dechanneling
4. Volume reflection
5. Volume capture
6. No effect



W. Scandale et al., PRL 98, 154801 (2007)

High-energy coherent phenomena in crystals



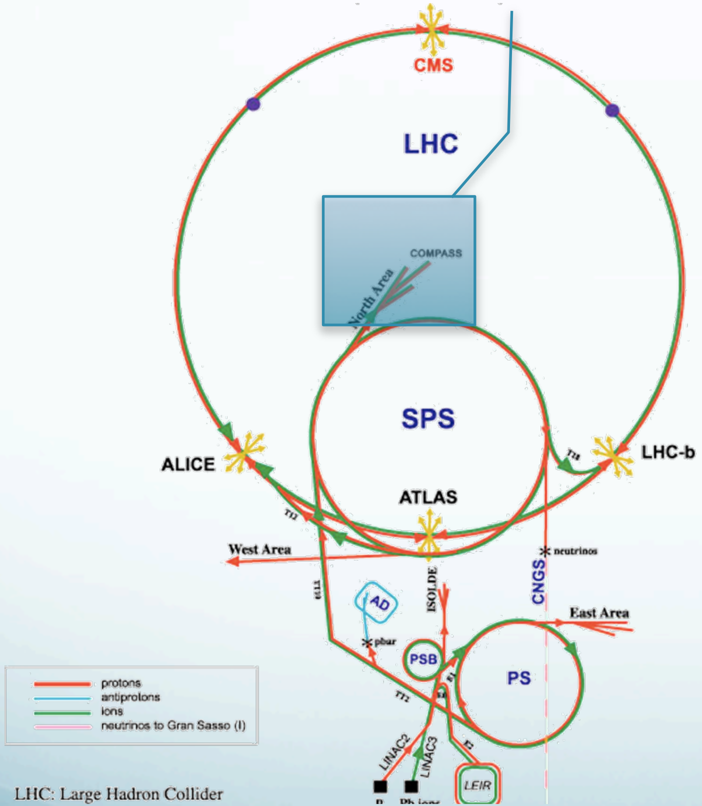
Experiments

H8 – protons 400 GeV/c

H4 – π^- 150 GeV/c

Experiments

CERN SPS H8/H4 lines



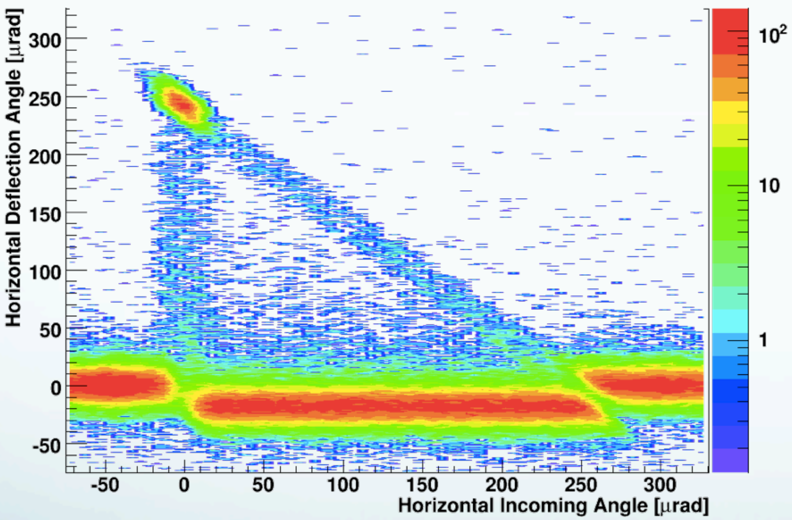
Experiments

- H4 Data-Taking:
  - 150 GeV/c π^-
  - from 27 June to 07 July
- H8 Data-Taking:
  - 400 GeV/c protons
  - From 09 July to 18 July
- Setup
  - Si-detector tracking system
    - 1 µrad angular resolution
  - High-resolution goniometer
    - 2 µrad resolution

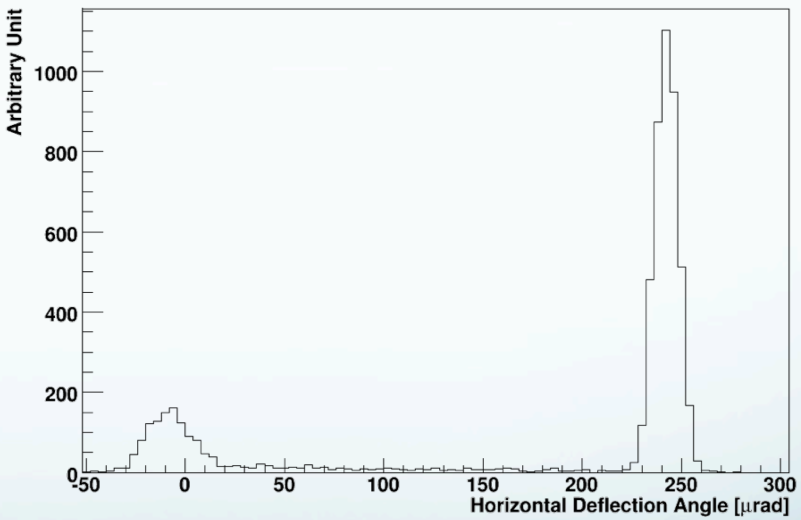
H8 – protons 400 GeV/c

Ge bent strip

Channeling efficiency

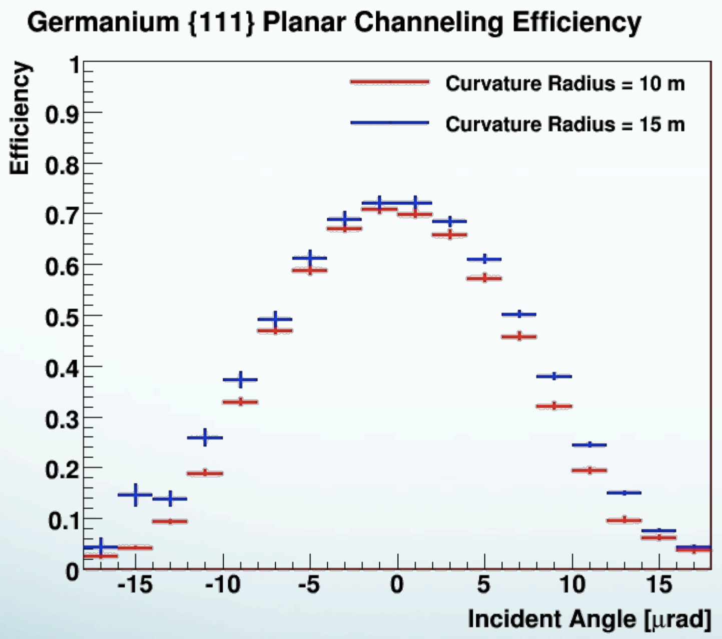


Deflection distribution

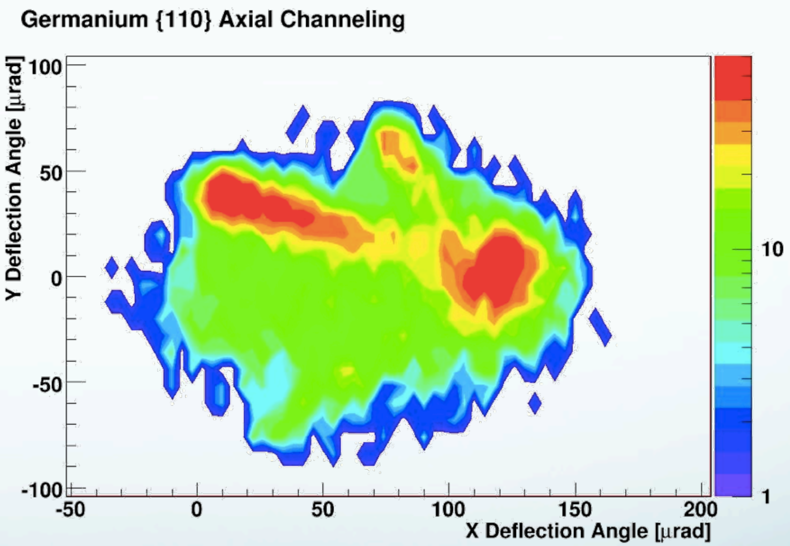


Ge bent strip

Efficiency

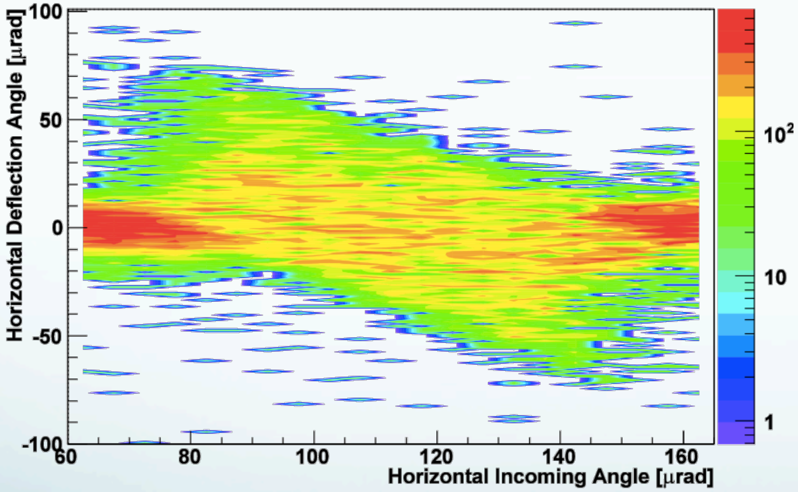


Axial channeling



Si crystalline undulator

Goniometer scan



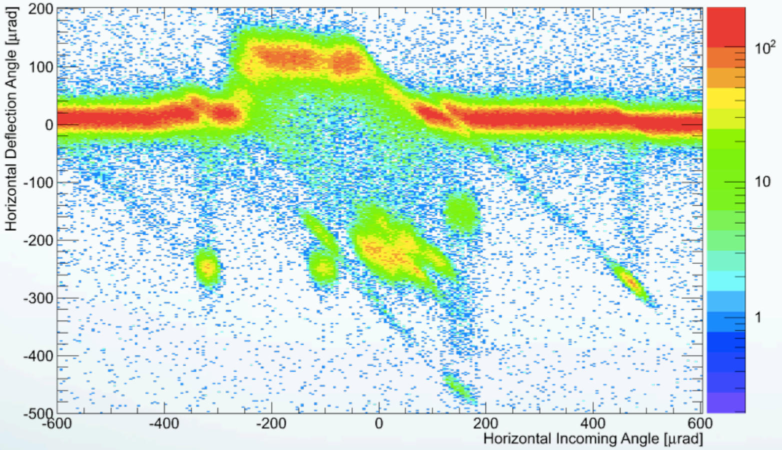
Undulator

- Fabricated in the Sensor and Semiconductor Lab (UniFE)
- Mechanically bent through grooves.
- Experimental evidence of double-sided bending.

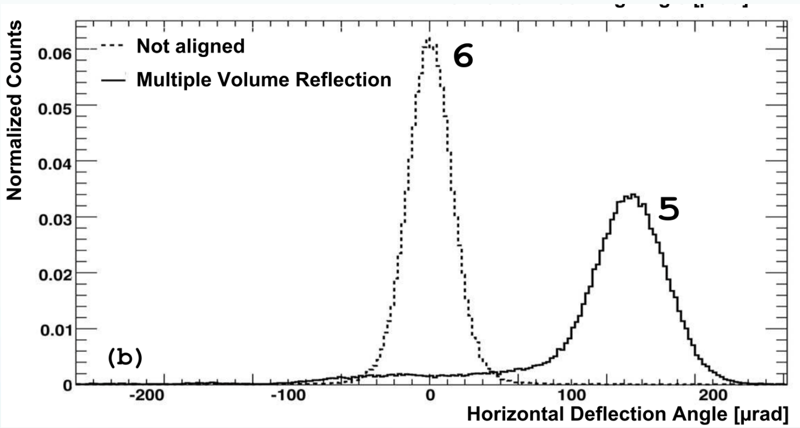
under analysis

Multi-crystals

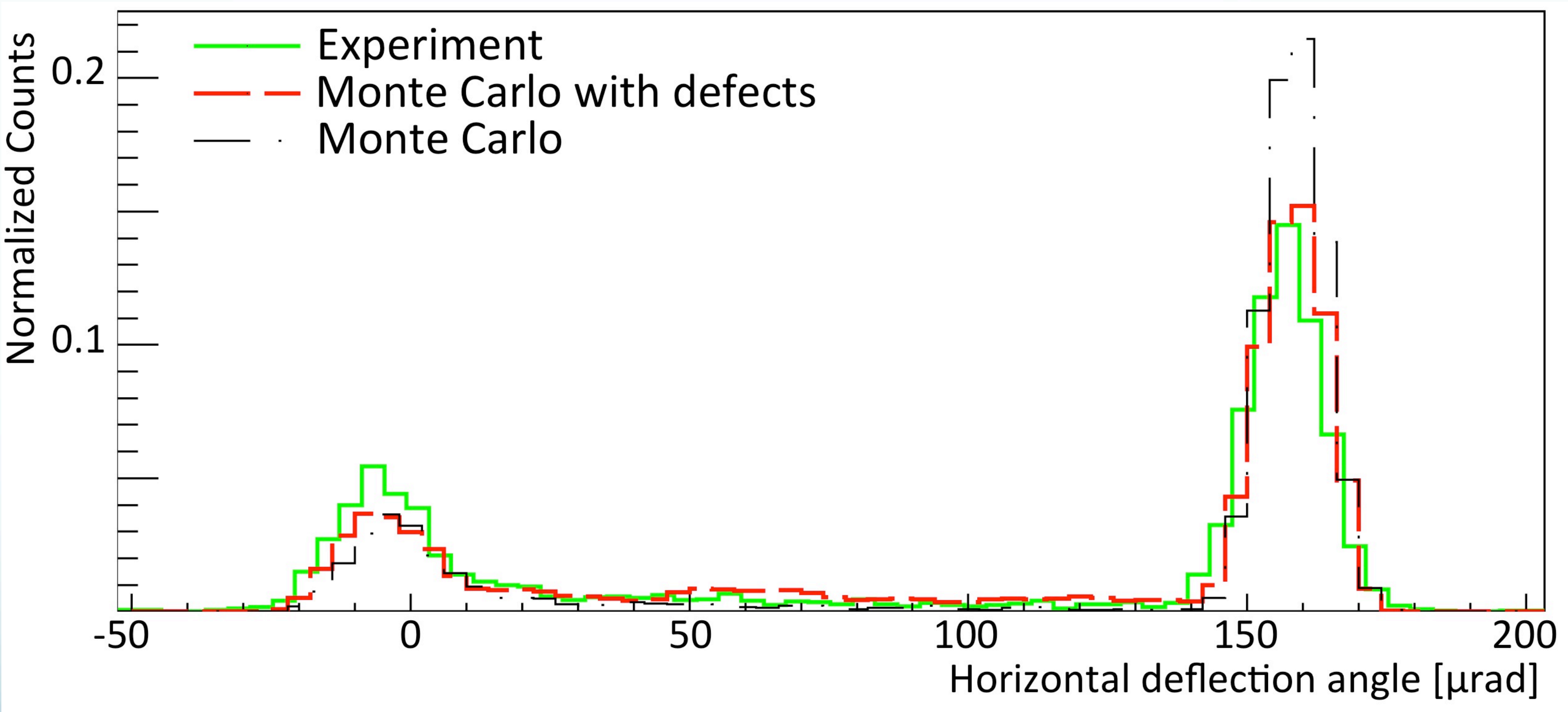
Goniometer scan



Profile MVR



SiGe self-bent crystal

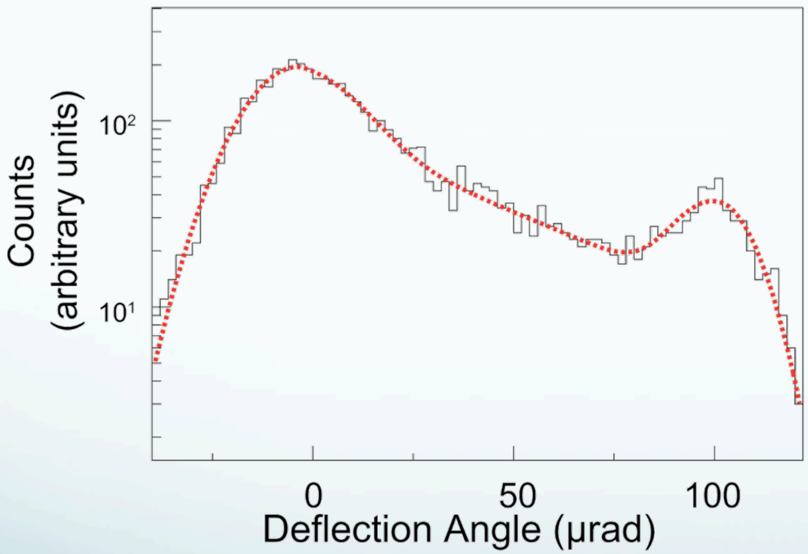


- SiGe self bent crystal
- (1 1 1) plane
- 25.6 m curvature radius
- 400 GeV/c proto
- defects

H4 – π^- 150 GeV/c

Dechanneling length

Deflection distribution



Dechanneling length

- First direct experimental measurement.
- Linear correlation between deflection angle and dechanneling point.
- Definition of simple equation to evaluate deflection efficiency.

Monte Carlo

DYNECHARM++
DYNECHARM++_Phi
Geant4 Channeling

DYNECHARM++

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INFN

Goals

- Physic goal:
  - Simulation of the orientational interactions between particles and crystals;
  - Correct reproduction of existing experimental data
  - Prediction of new experiments and phenomena.
- Programming goal:
  - Fast;
  - Expandable;
  - Easily updatable;
  - Linkable.

Method

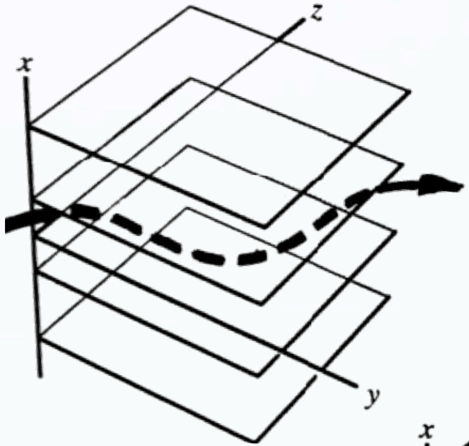
- Two Monte Carlo methods:
  - Simulation: integration of the equation of motion for every particle;
  - Emulation: usage of cross section to describe orientational phenomena.

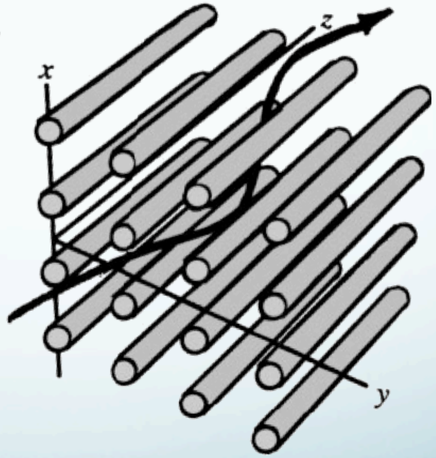
Method

- C++ language
  - Widespread programming language in high-energy physic community (ROOT, Geant4, etc...);
  - Object oriented programming language;
  - Compile on almost all systems;
  - Exploit parallelization at all level.

Continuum potential approximation

- Particle impinge on a crystal close to atomic planes or axes.
- Particle "sees" aligned atoms as a unique axis.
- Aligned axes form planes.
- Particle interaction with atoms can be approximated through interaction with atomic planes or axes [1].





J. Lindhard, Danske Vid. Selsk. Mat. Fys. Medd. 34, 14 (1965)

Continuum potential calculation

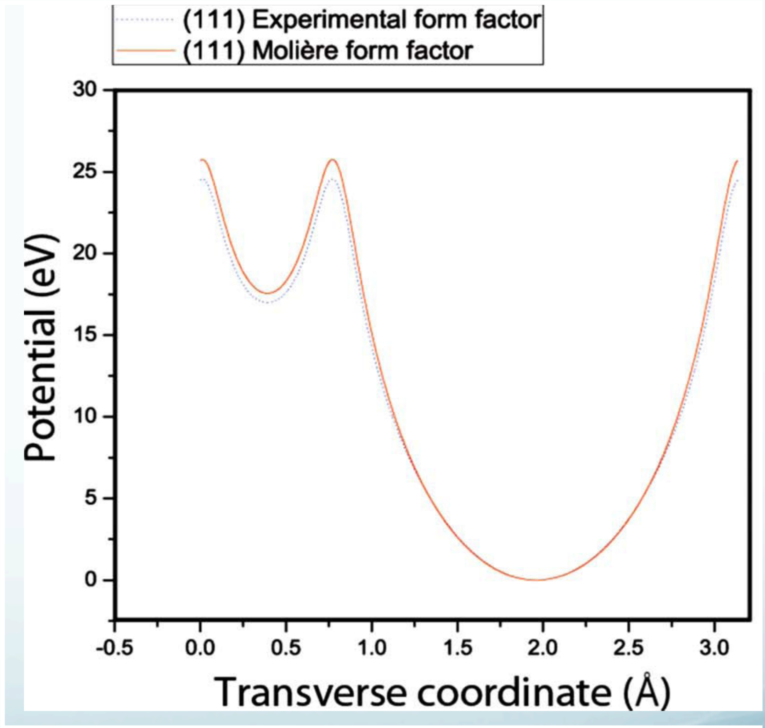
ECHARM

- Calculation method based on the expansion of the electrical characteristics of crystals in Fourier series.

$$\varphi(\mathbf{r}) = \frac{4\pi e}{\Delta} \sum_{g \neq 0} \sum_{l=1}^{N} Z_l S(Z_l, \mathbf{g}) \frac{[1 - F(Z_l, g)]}{g^2} e^{-i\mathbf{g}\cdot\mathbf{r}}$$

- Electrical characteristics are averaged over planar and atomic.
- Different approximation for atomic form factor.
- Approximation for any planes or axes for cubic structure.

Si (111) Planar Potential



E. Bagli, V. Guidi, V. Maisheev, Phys. Rev. E 81, 026708 (2010)

Emulation method

- Analytical approximations [1,2] and experimental data [3,4] to calculate the cross section of the phenomena.
- Less computational time than integration of the equation of motion.
- Theoretical knowledge of orientational planar phenomena has been largely verified through results to be treated via a macroscopic approach.
- It can be used to simulate known crystal effects, but can not be used to predict strange or new phenomena

[1] V.M. Biryukov, Y.A. Chesnokov and V.I. Kotov, *Crystal channeling and its application at high-energy accelerators*, Springer-Verlag, Berlin Germany (1997).
[2] V.A. Maisheev, *Phys. Rev. ST Accel. Beams* 10 (2007) 084701 [physics/0607009].
[3] Y.M. Ivanov et al., *Phys. Rev. Lett.* 97 (2006) 144801

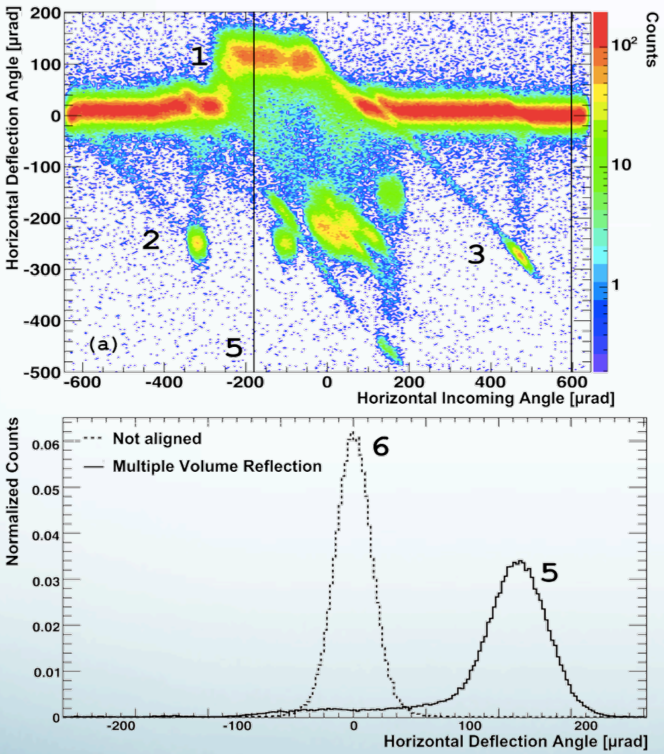
Simulation method

- Integration of the equation of particle motion through Velocity-Verlet numerical method [1].
- Electric field experienced by particles in the interaction with the oriented crystal is evaluated through continuum potential approximation [2].
- Transverse energy variation due to interaction with electrons and nuclei is taken into consideration through Kitagawa and Ohtsuki approximation [3] applied to multiple scattering approximation [4].
- Possibility to add crystal defects to the simulation.

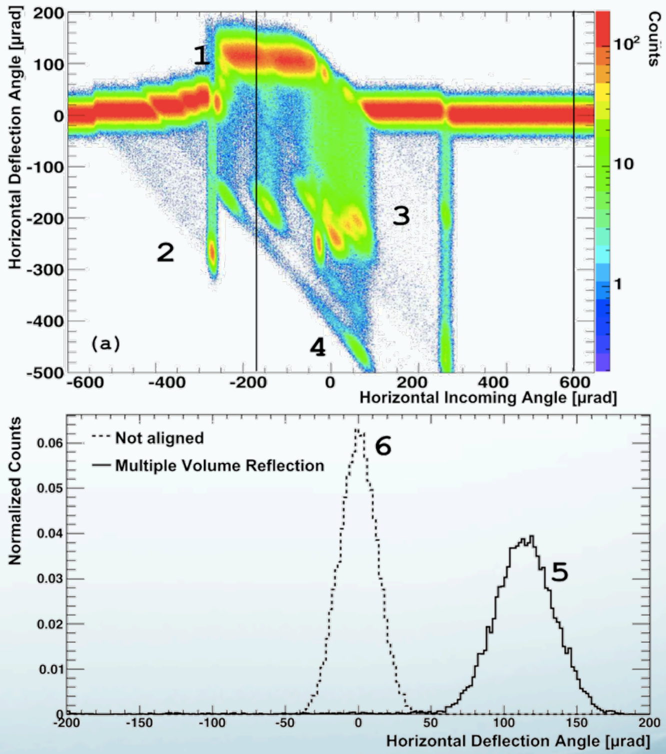
[1] L. Verlet, Phys. Rev. 159, 98 (1967); Phys. Rev. 165, 201 (1967)
[2] J. Lindhard, Danske Vid. Selsk. Mat. Fys. Medd. 34, 14 (1965)
[3] M. Kitagawa and Y. H. Ohtsuki, Phys. Rev. B 8, 3117–3123 (1973)
[4] J. Beringer *et al.* (Particle Data Group), Phys. Rev. D86, 010001 (2012)

Multi-crystal

COHERENT [1]



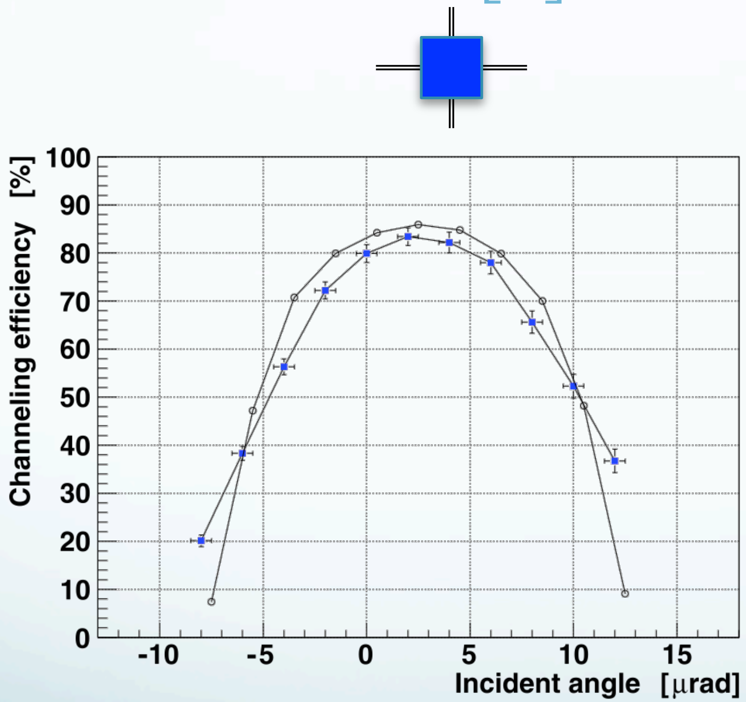
DYNECHARM++



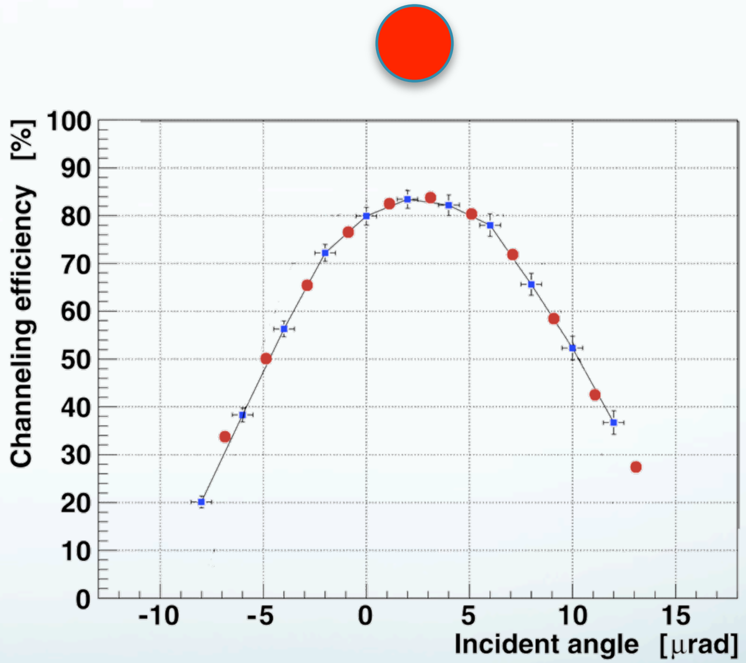
[1] E. Bagli *et al.*, JINST, 7, P04002 (2012)

Si-efficiency simulation

H8RD22 [1]



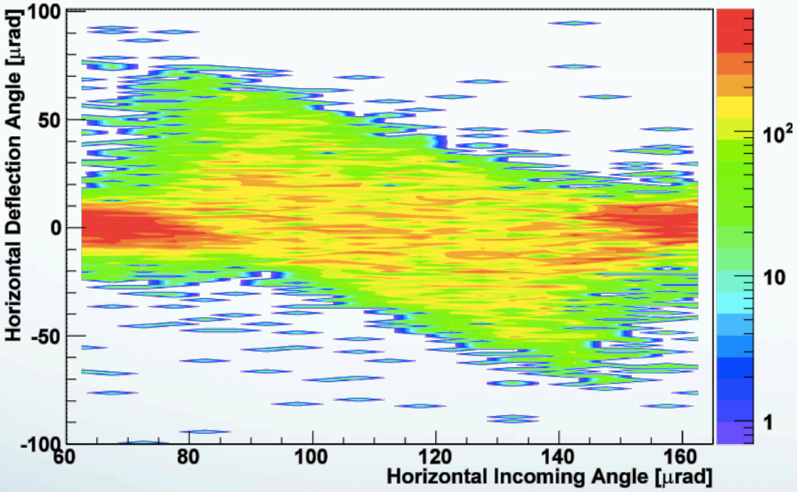
DYNECHARM++



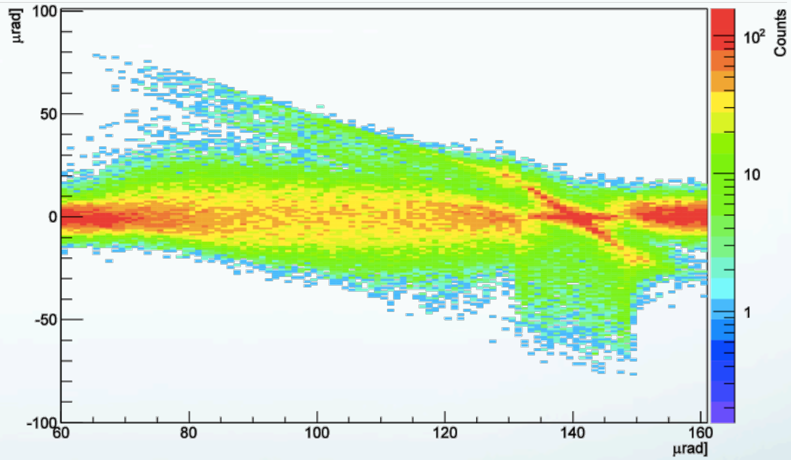
[1] W. Scandale *et al*, Phys. Lett. B, 680, 129 (2009)

Si crystalline undulator

COHERENT [1]

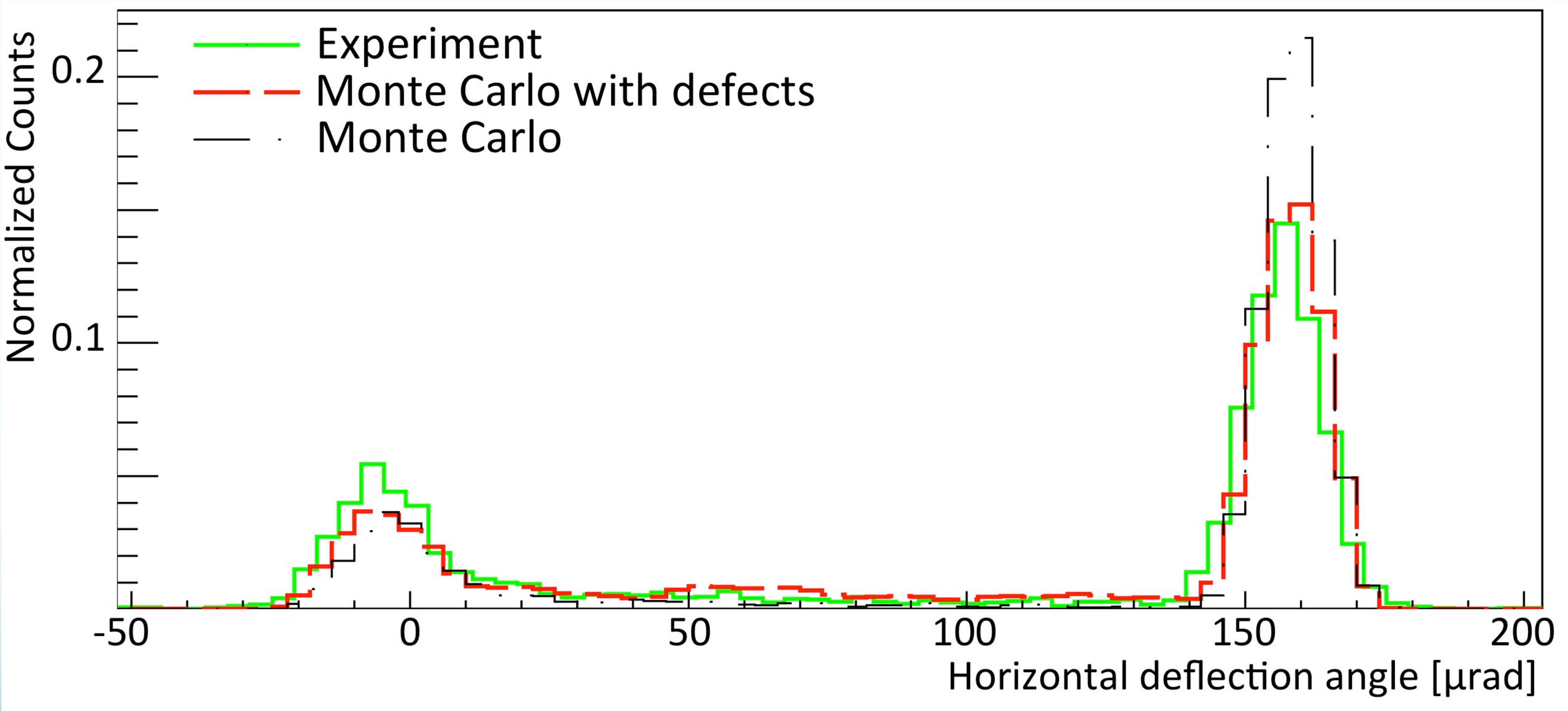


DYNECHARM++



[1] COHERENT experiment, not published

SiGe self-bent crystal



- SiGe self bent crystal
- (1 1 1) plane
- 25.6 m curvature radius
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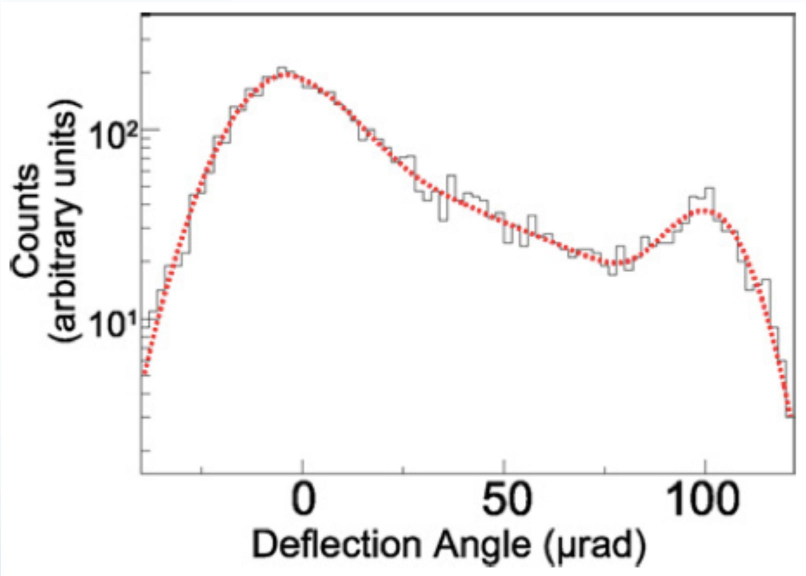
Dechanneling length



Experiment

- $L = (0.93 \pm 0.05)$ mm
- $\varepsilon_{ch} = (12.5 \pm 1.0)$ %

DYNECHARM++

- $L = (0.95 \pm 0.03)$ mm
- $\varepsilon_{ch} = (14.3 \pm 0.3)$ %

DYNECHARM++_Phi

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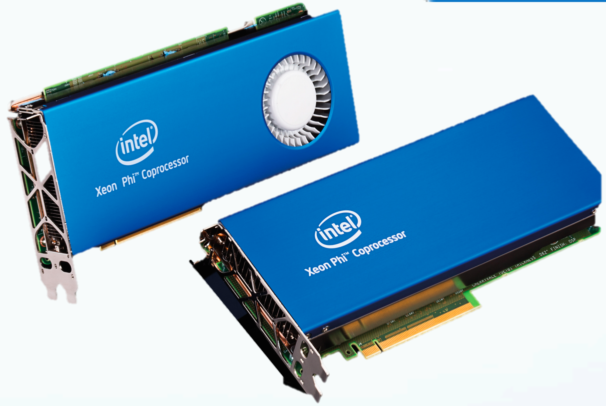
Colfax International

Xeon Phi™ 5110P

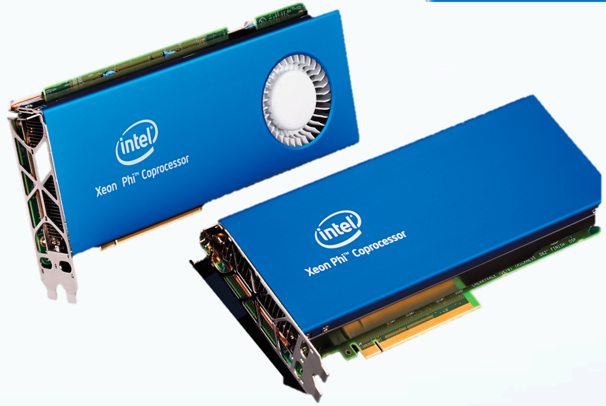
- 60 cores (240 with Hyper-threading)
- 1.053 GHz clock
- 8 GB on-board memory
- AVX-512 register scheme
- PCIe card form factor
- Up to 8 cards in parallel



Colfax International

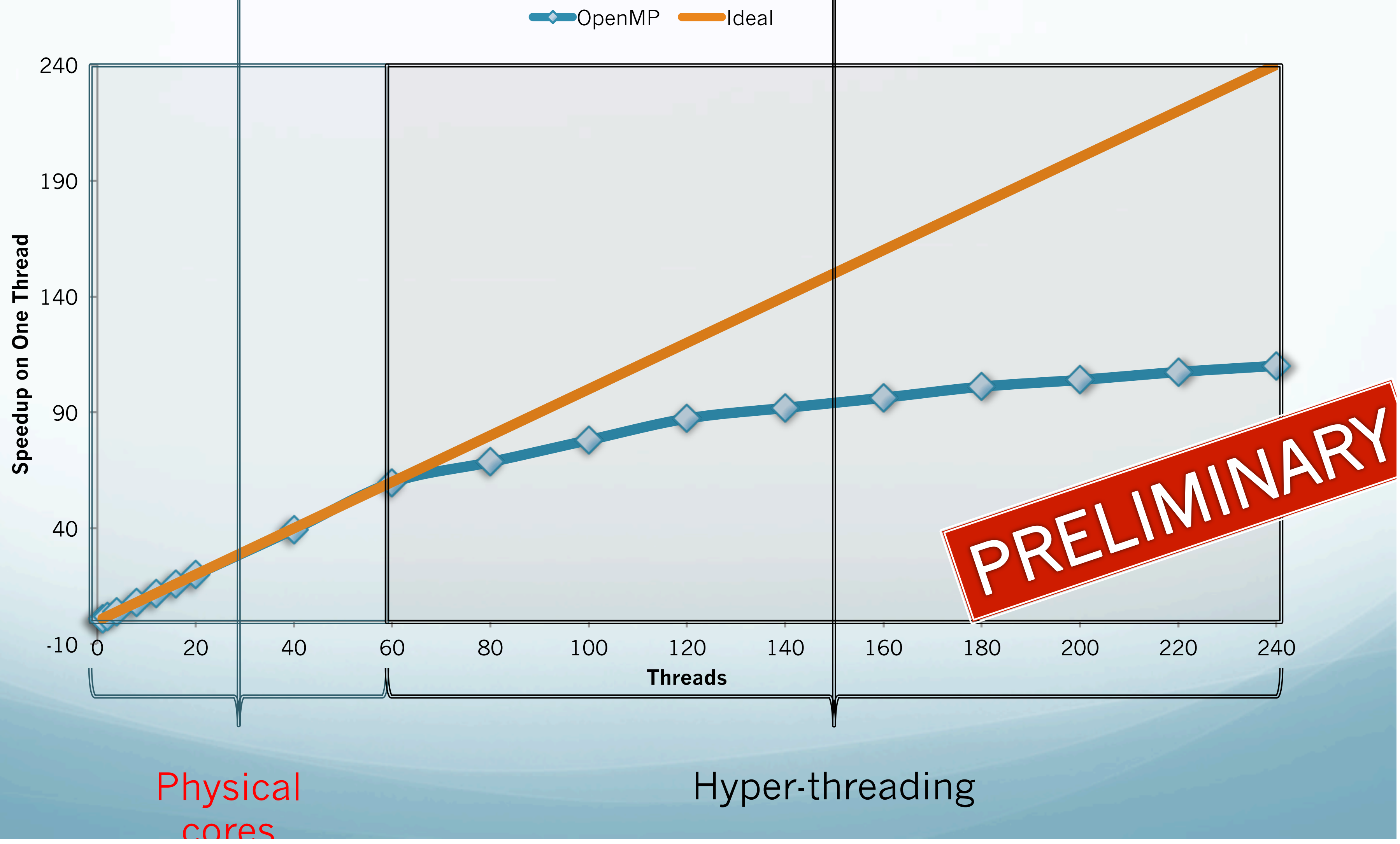
DYNECHARM++ code has been revised to exploit parallelization at two levels:

- Multithreading on 240 and more cores
- Vectorization on 512-bit wide register

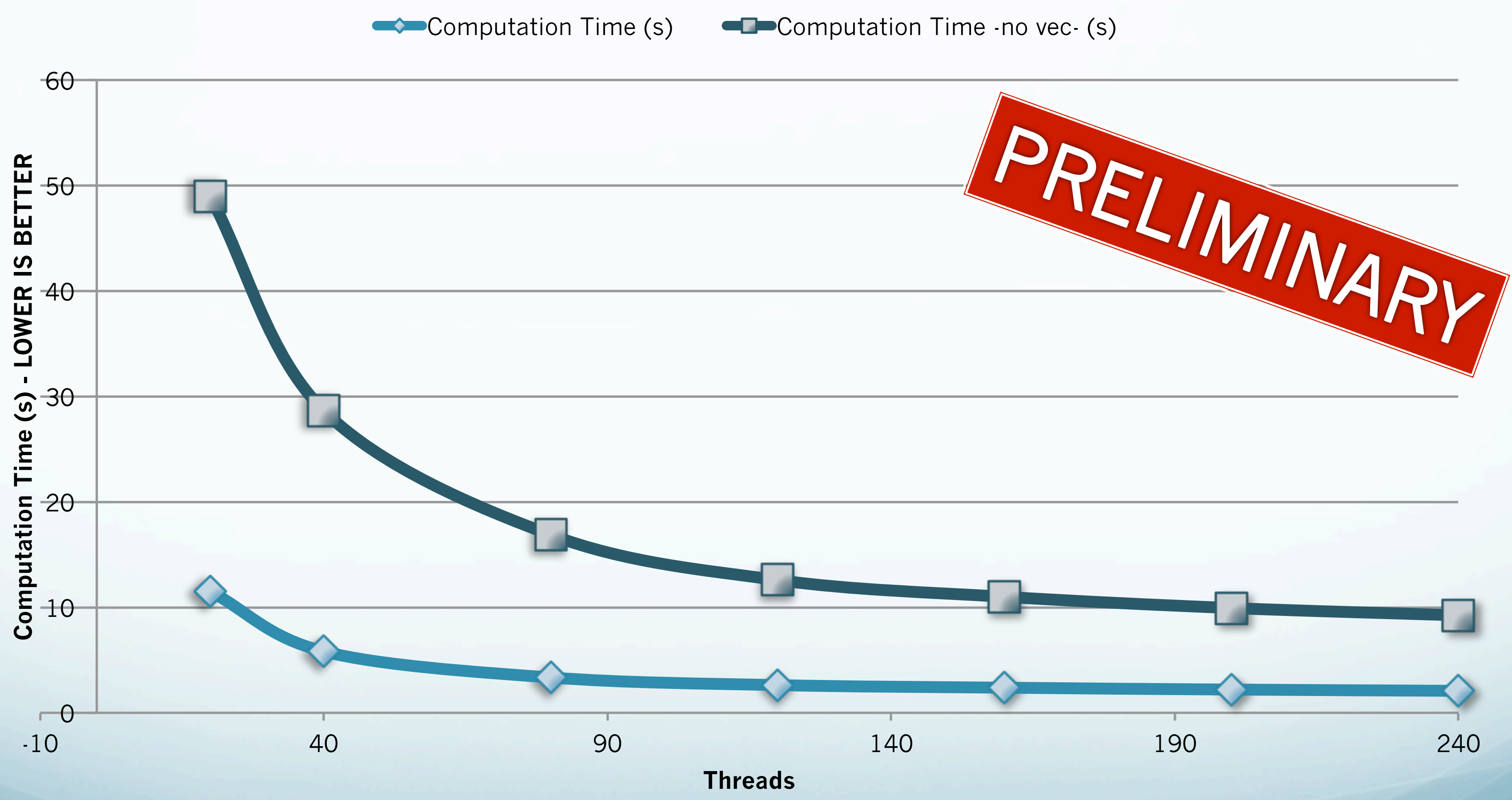


Colfax International

Multithreading

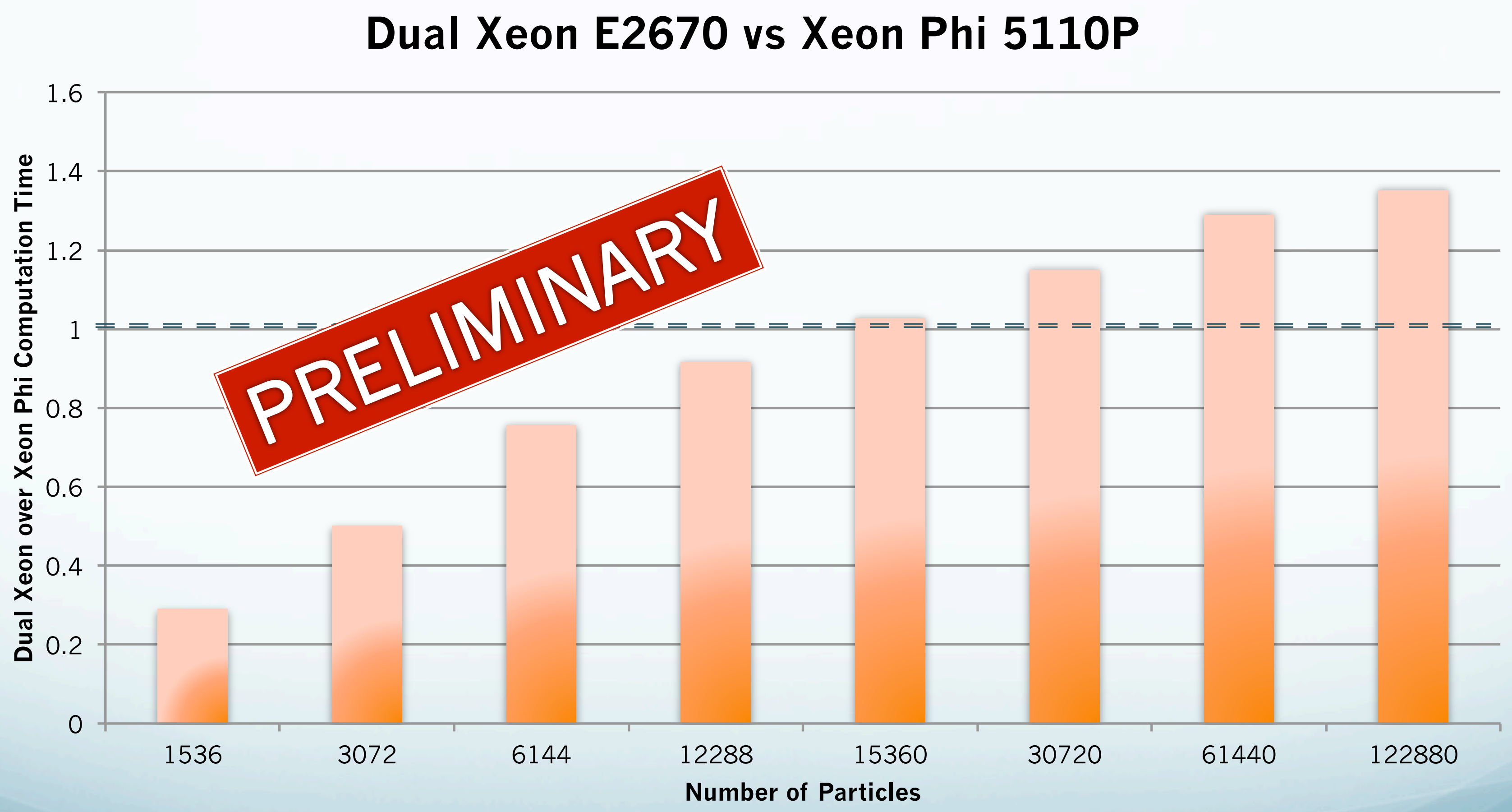


Vectorization



15360
Particles

Xeon vs. Xeon Phi



- - - - Same computation time

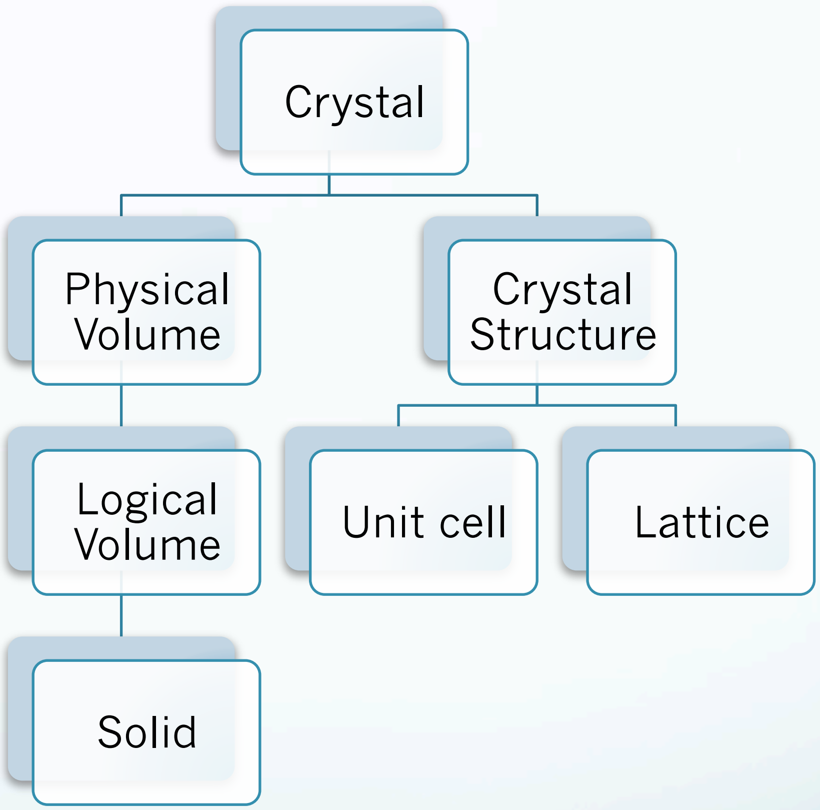
Geant4 Channeling

Motivation

- *"Geant4 is a toolkit for the simulation of the passage of particles through matter. Its areas of application include high energy, nuclear and accelerator physics, as well as studies in medical and space science."*
- In October 2012 the first Geant4 release with support for crystal structures was released.
- Implementation of channeling into Geant4 can lead to:
  - evaluation of channeling influence on current simulation made with Geant4
  - addition of the Geant4 toolkit advantages to the simulation of current and new experiments based on channeling (e.g. beam collimation and extraction with crystal)

Crystal

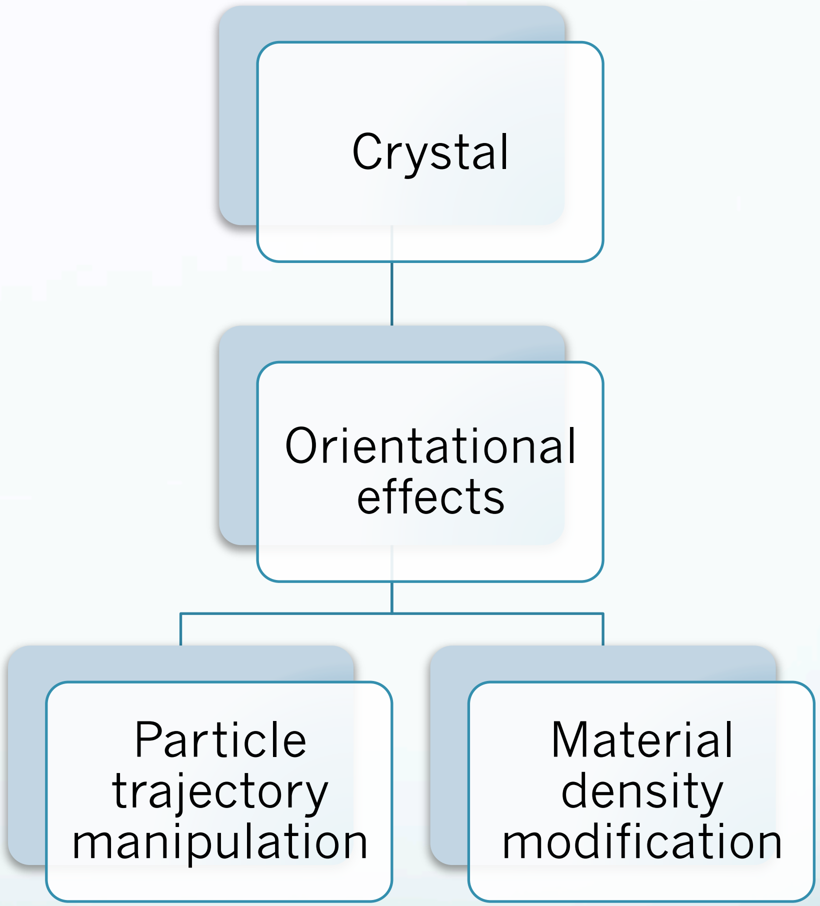
The crystal object is built adding to the standard Physical Volume the Crystal Structure in which the Unit Cell and the Lattice are defined.



Geant4 processes modification

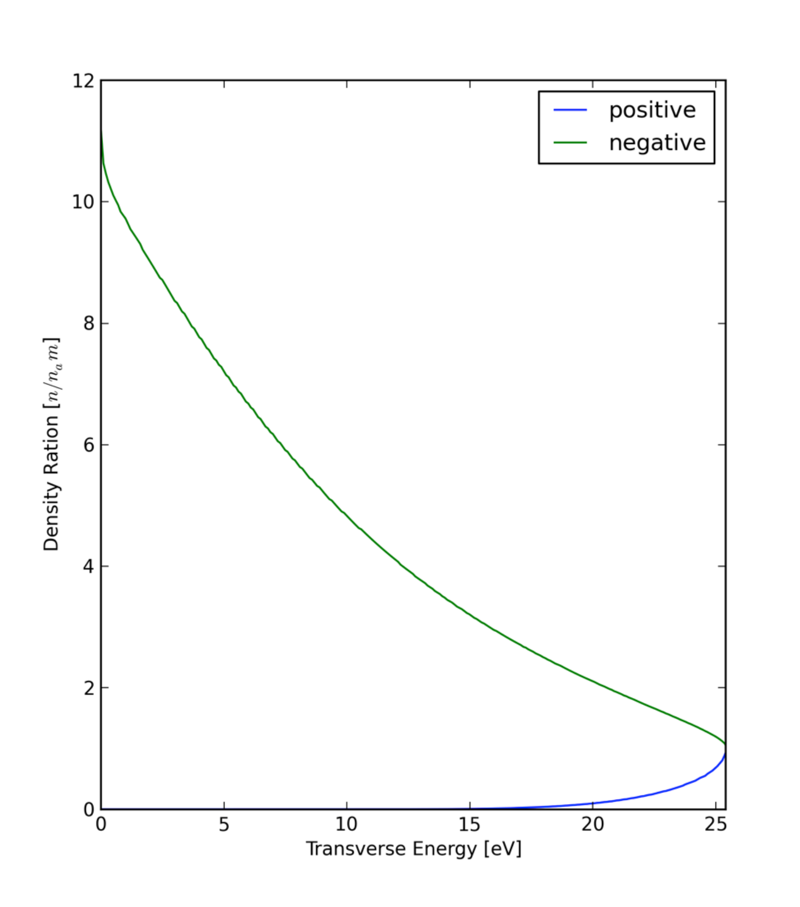
By modifying the trajectory of the particle and the density of the material "seen" by the particle the orientational effects in a crystal affect all the Geant4 physical process

As an example channeled positive particles oscillate between atomic planes interacting less frequently with nuclei and core electrons.



Modified density

- Nuclei and electron density tables are computed for positive and negative particles as a function of the particle transverse energy.
- This approach can be used for crystal with dimension parallel to the beam much longer than the channeling oscillation period.



Geant4 processes

Discrete processes

- The mean free path of the discrete processes is recomputed at each step using the modified density because it is directly proportional to the density (ρ) of the material.

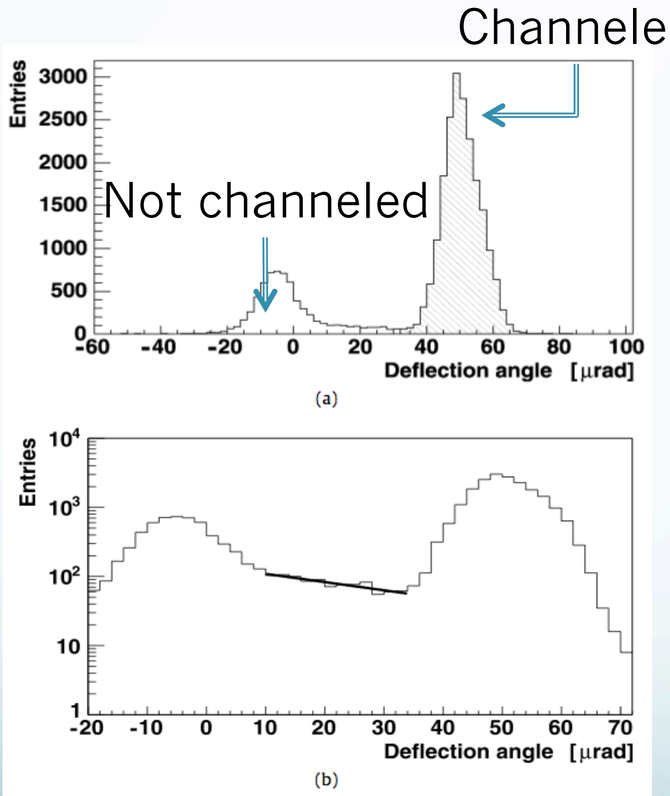
Continuous processes

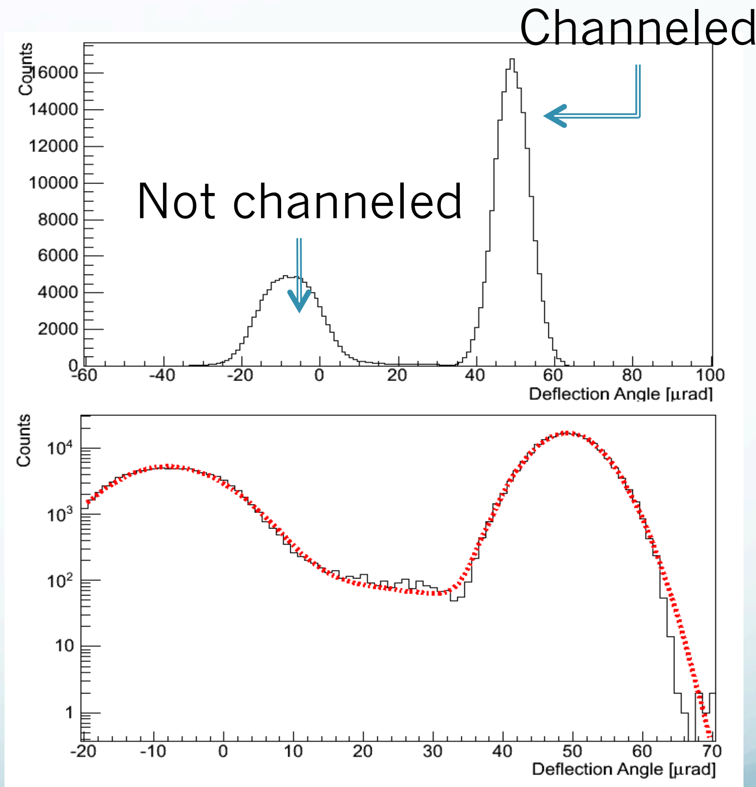
- Material density (ρ) for the calculation of continuous energy loss (dE/dx) is modified at each step (dx=ρ dz) to enable the reduction or the enhancement of the energy loss due to channeling.

Nuclear dechanneling length

W. Scandale et al., Phys. Lett. B 680 (2009) 129

Geant4 Channeling



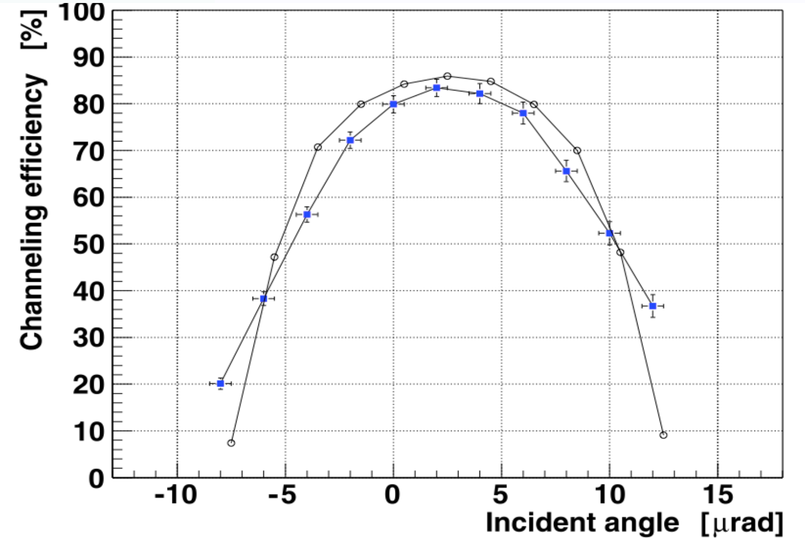


$L_n = (1.53 \pm 0.35 \pm 0.20)$ mm

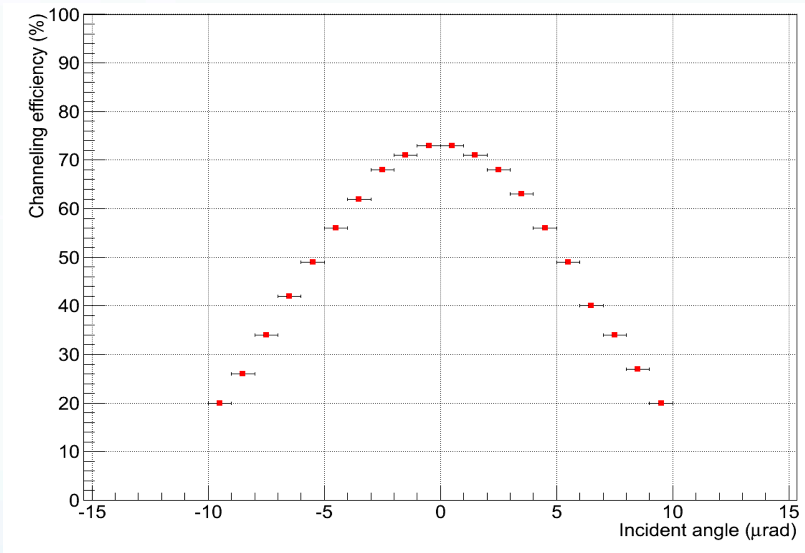
$L_n = (1.31 \pm 0.05)$ mm

Channeling efficiency vs. incoming angle

W. Scandale et al., Phys. Lett. B 680 (2009) 129



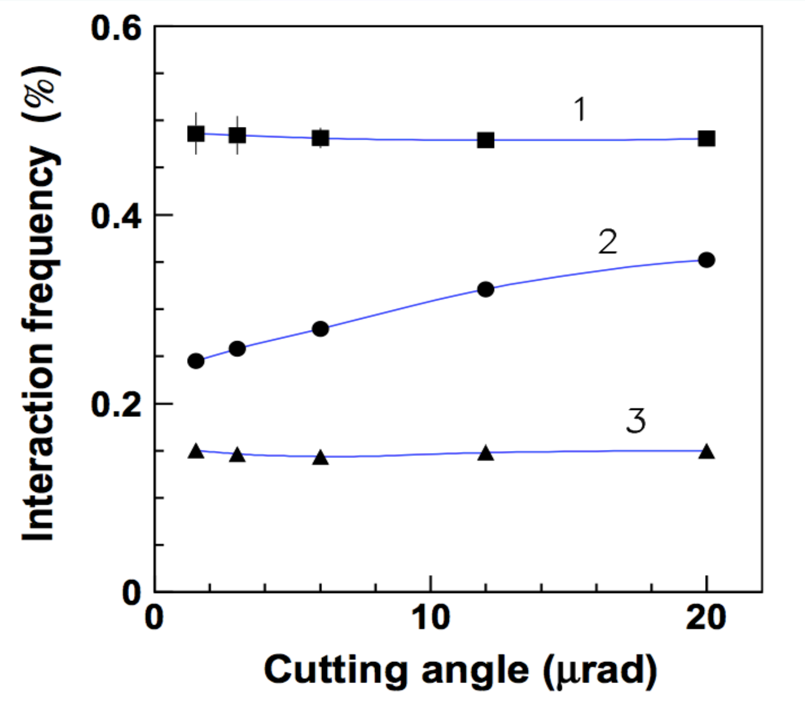
Geant4 Channeling



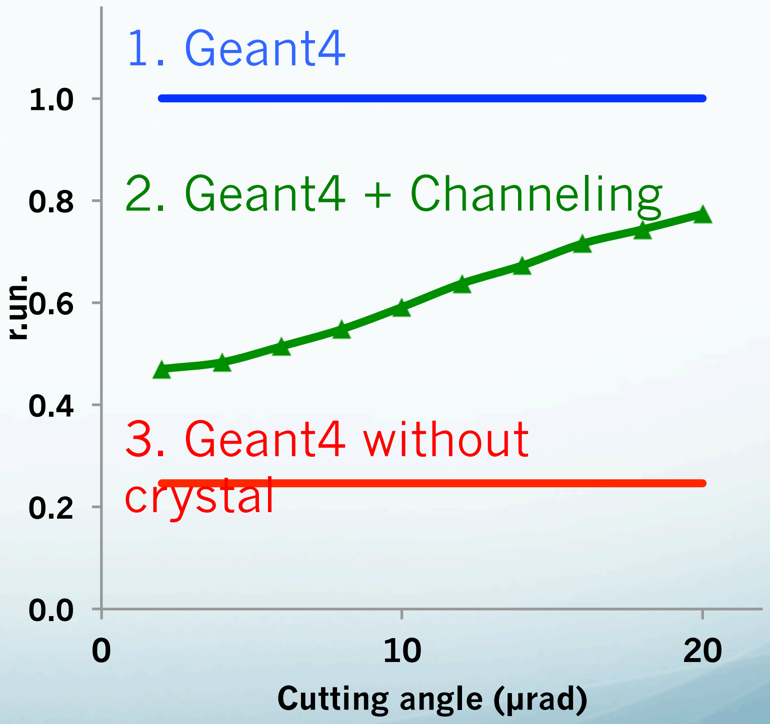
- Experimental measurements (a)
- UA9 collaboration simulations (a)
- Geant4 Simulations (b)

Interaction rates vs. integration angle

W. Scandale et al., NIMB 268 (2010) 2655

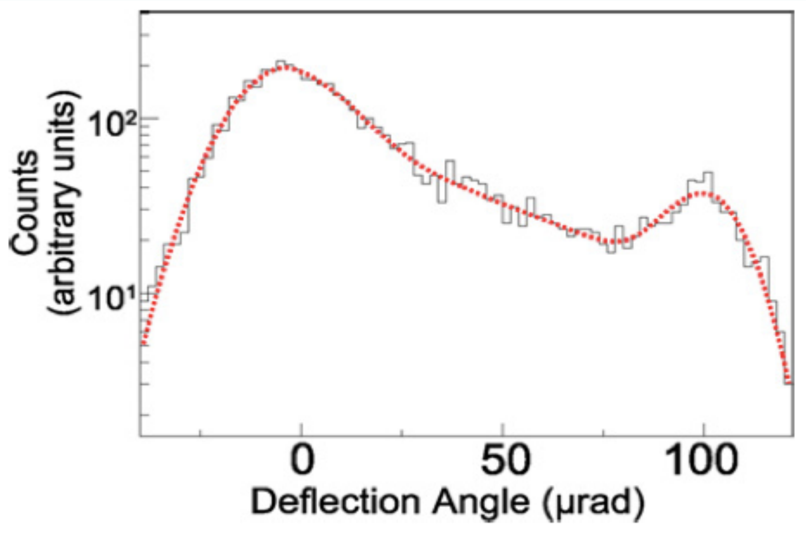


Geant4 Channeling



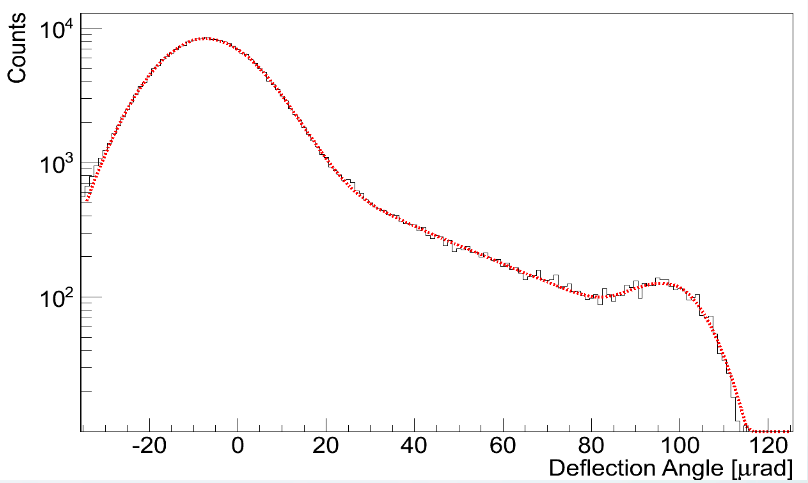
Dechanneling length for π⁻

W. Scandale et al., Phys. Lett. B 680 (2009) 129



L = (0.93 ± 0.05) mm
ε_{ch} = (12.5 ± 1.0) %
θ_{ch} = (99.6 ± 0.2) μrad

Geant4 Channeling



L = (0.60 ±- 0.05) mm
ε_{ch} = (4.5 ± 0.2) %
θ_{ch} = (95.6 ± 0.6) μrad

Conclusions

- Experiments of orientational effects for positive and negative particle in bent crystals, multi-crystals, Si and Ge crystals, SiGe self-bent crystals, crystalline undulators.
- Monte Carlo simulation of particle trajectories in crystals (DYNECHARM++)
- Exploitation of modern computational technologies (DYNECHARM++_Phi)
- Implementation of orientational effect in the most used Monte Carlo code for particle physics (Geant4 Channeling)

Thank you for the attention